

The Merck Index Online[™]

FILE DESCRIPTION

The Merck Index OnlineSM is the online version of the monographs in the printed 12th Edition of *The Merck Index* (a U.S. publication, Whitehouse Station, N.J., USA), an internationally recognized, one-volume encyclopedia of chemicals, drugs, and biologicals. Each monograph in the encyclopedia (each record in the database) discusses a single chemical entity or a small group of very closely-related compounds. Updates contain material not yet available in print.

Records contain molecular formulas and weights, systematic chemical names (including CAS names), generic and trivial names, brand names and their associated companies, company codes, CAS Registry numbers, physical and toxicity data, therapeutic and commercial uses, and bibliographic citations to the chemical, biomedical, and patent literature.

SUBJECT COVERAGE

The database includes, but is not limited to, monographs on the following types of compounds:

- Agricultural chemicals (including pesticides and herbicides)
- Biological products
- Environmentally significant compounds
- · Human drugs
- Natural products
- Organic and inorganic chemicals used in commerce and research
- Veterinary drugs

SOURCES

Records contain information from and citations to approximately 700 international chemical, biomedical, and clinical journals; patents issued by more than 20 countries; books; proceedings; and other standard reference works.

DIALOG FILE DATA

Inclusive Dates: Late 19th Century to the present

Update Frequency: Semi-Annual

File Size: 10,430 records as of February 1998

CONTACT

The Merck Index Online is produced by Merck & Co., Inc., Whitehouse Station, NJ, USA. Questions concerning file content should be directed to:

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The Merck Index Onlinesm

DIALOG(R)File 304: The Merck Index Online(SM) (c) 1996,1997 MERCK & CO. INC. All rts. reserv.

AN=JMN,MN=JDEJNA,NA=JMAINRN= MF=, MW=

/CN, CN=, /NA, NA=, /DE

/SY, SY=, /NA, NA=, /DE

/S0, SO=

Monograph Name: Enalapril CAS REGISTRY NUMBER: 75847-73-3 MOLECULAR FORMULA: C20H28N2O5 MOLECULAR WEIGHT: 376.45 MOLECULAR COMPOSITION: C 63.81%, H 7.50%, N 7.44%, O 21.25% C.A. CHEMICAL NAME(s): (S)-1-(N-(1-(Ethoxycarbonyl)-3-phenylpropyl)-L-alanyl)-L-proline 1-(N-((S)-1-carboxy-3-phenylpropyl)-L-alanyl)-L-proline

LITERATURE REFERENCES: Angiotensin-converting enzyme (ACE) inhibitor; de-esterified in vivo to its active diacid metabolite, enalaprilat, q.v. Prepn: A. A. Patchett et al., Nature 288, 280 (1980); eidem, Eur. pat. Appl. 12,401; E. E. Harris et al., U.S. pat. 4,374,829 (1980, 1983 both to Merck & Co.). Pharmacology: D. M. Gross et al., J. Pharmacol. Exp. Ther. 216, 552 (1981); C. S. Sweet et al., ibid. 558.

Bioavailability and metabolism: E. H. Ulm, Drug Metab. Rev. 14, 99 (1983). Comprehensive description: D. P. Ip, G. S. Brenner, Anal. Profiles Drug Subs. 16, 207-243 (1987). Clinical trial in congestive heart failure: Consensus Trial Study Group, N. Engl. J. Med. 316, 1429 (1987). Review of clinical experience in hypertension: H. J. Gomez et al., J. Cardiovasc. Pharmacol. 15, Suppl. 3, S26-S29 (1990); of clinical pharmacokinetics: R. J. MacFadyen et al., Clin. Pharmacokinet. 25, 274-282 (1993); of combination with hydrochlorothiazide: P. L. Malini, Adv. Ther. 10,

253-262 (1993). PATENT INFORMATION:

EP 12401; US 4374829 DERIVATIVE INFORMATION:

SUBSTANCE: Enalapril Maleate DERIVATIVE CAS RN: 76095-16-4

DERIVATIVE MOL. FORMULA: C20H28N2O5.C4H4O4 DERIVATIVE DRUG CODES: MK-421

DERIVATIVE BRAND NAME (COMPANY): Amprace (Amrad), Bitensil (UCB), Cardiovet (Intervet), Enacard (Merck & Co.), Enaloc (Leiras), Enapren (Merck & Co.), Glioten (Bago), Hipoartel (Lasa), Innovace (Merck & Co.), Lotrial (Roemmers), Olivin (Lek), Pres (Dieckmann), Renitec (Merck & Co.), Reniten (Merck & Co.), Renivace (Banyu), Vasotec (Merck & Co.), Xanef (Merck & Co.)

DERIVATIVE PHYSICAL DATA: White to off-white crystalline powder, mp 143-144.5 degrees. Soly (g/ml): water 0.025; alcohol 0.08; methanol 0.20. (.alpha.)D25 -42.2 degrees (c = 1 in methanol). pH (1% water) 2.6. pKal 3.0; pKa2 (25 degrees) 5.4. MELTING POINT: 143-144.5 degrees

OPTICAL ROTATION: (.alpha. D): -42.2 degrees (c = 1 in methanol) SUBSTANCE: Enalapril Mixture of maleate with hydrochlorothiazide DERIVATIVE BRAND NAME (COMPANY): Acesistem (Sigma-Tau),

Co-Renitec (Merck & Co.), Innozide (Merck & Co.), Renacor (Merck & Co.), Vaseretic (Merck & Co.), Xynertec (Merck & Co.)
THERAPBUTIC CATEGORY: Antihypertensive.

THERAPEUTIC CATEGORY VET: In treatment of heart failure in dogs. REFERENCE KEYS PRESENT: Clinical trial; In Vivo; Patent number; Pharmacology; Prepn; Review

DATA KEYS PRESENT: Molecular weight; Patent number; Therap. Cat.; Therap. Cat. Vet.

DATA KEYS PRESENT IN DERIVATIVE: Melting point; Optical rotation

PN =/DERIV /SY, SY=, /NA, NA=, /DE RN= MF =/SY, SY=, /NA, NA=, /DE /TN, TN=, /SY, SY=, /NA, NA=, /DE

/C0, CO=

/PP, PP=

MP=, MT= OP=, OT=/SY, SY=, /NA, NA=, /DE /TN, TN=, /SY, SY=, /NA, NA=,/DE/CO, CO= /TC, TC= /TC, TV=

/DP, RP= /DP, DP=

/DP, DP=, /DERIV

SEARCH OPTIONS

BASIC INDEX

SEARCH SUFFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
/CN	CN	All Basic Index Fields CA Chemical Name ^{1,2}	Word Segment & Word &	S ETHOXYCARBONYL(1W)PHENYLPROPYL S PROPYL/CN S
/CO /DE	CO DE	Company Name ¹ Chemical Name	Phrase Word Segment & Word &	ETHOXYCARBONYL(1W)PHENYLPROPYI S "S)-1-(N-(1-(ETHOXYCARBONYL)-3"?/CN S MERCK/CO S PHENYL/DE
/DP /EC /MN	DP MF MN	Data Present ^{1,3} Element Count ² Monograph Name ¹	Phrase Word Phrase Segment &	S ENALAPRIL(W)MALEATE/DE S ENALAPRIL MALEATE/DE S MELTING(W)POINT S (C20(S)N2)/EC S CHLORIDE/MN
'NA	NA	Chemical Name ¹	Word & Phrase Segment & Word &	S ENALAPRIL/MN S ANTIMONY TRICHLORIDE/MN
NT PP	NT PP	Notes and Cautions	Phrase Word	S ENALAPRIL MALEATE/NA
so	so	Physical Property Information ³ Sources/References ⁴	Word Word	S MORDANT(S)CATALYST/NT S WHITE(1W)POWDER/PP
SY	SY	Synonyms Including Brand Names and Drug Codes 1.2	Segment & Word &	S ACADEMIC(W)PRESS/SO S U(W)S(W)PAT?/SO S AL/SY,DERIV S CO(W)RENITEC/SY
	TC TN	Therapeutic Category ⁶ Brand Name ^{1,2}	Phrase Word Segment &	S CO-RENITEC/SY S ANTIHYPERTENSIVE/TC S AL/TN S LOTRIAL/TN,DERIV
Searchable		Index and in the Additional Indexes Apy 4		S CO-RENITEC/TN

Searchable in the Basic Index and in the Additional Indexes. Any numeric values are searchable in the Basic Index using the (W) operator, e.g. S 143(W)144(W)5/PP

ADDITIONAL INDEXES

PREFIX	DISPLAY	FIELD NAME	INDEXING	SELECT EXAMPLES
AN= AN= BP= BT= CN= CO= DN= DP= DT= EC=	CODE AN AN BP BP CN CO DN DP DN MF	DIALOG Accession Number THE MERCK INDEX Monograph Number Boiling Point (Celsius) ^{1,7} Boiling Point Text ¹ C.A. Chemical Name ¹ Company Name ¹ Relative Density ^{1,7} Data Present ^{1,3} Density Text ¹ Element Count ¹		SELECT EXAMPLES S AN=03521 S AN=03521 S BP=223.5 S BT=DEGREES S CN=S)-1-(N-(1-(ETHOXYCARBONYL? S CO=MERCK & CO? S DN=1.0000 S DP=(BOILING POINT AND MELTING POINT) S DT=SUPERCOOLED AND DN=1.0 S EC=(C0020 AND H0028)
FF= FP= FT= LD= ME= MF= MN= MP= MT= MY= NA= OP= OT= PN=	MN MP MP MW NA OP OP PN	Flash Point (Fahrenheit) ^{1,7} Flash Point (Celsius) ^{1,7} Flash Point Text ¹ Lethal Dose (LD50) ¹ Molecular Elements Molecular Formula Monograph Name ¹ Melting Point Text ¹ Molecular Weight ⁷ Chemical Name ^{1,4} Optical Rotation ^{1,7} Optical Rotation Text ¹ Patent Number ¹ Physical Property Information ¹	Word Numeric Phrase Numeric Word Phrase	S EC=N0001:N0005 S FF=84.2 S FP=29 S FT=(CLOSED(W)CUP) S LD=(RATS AND S(W)C) S ME=CHNO S MF=C20H28N2O5 S MN=ENALAPRIL S MP=144 S MT=DEGREES S MW=376.45 S NA=ENALAPRIL S OP=10.1:10.9 S OT=(ALPHA(S)22(S)546) S PN=US 4374829 S PP=(OFF(W)WHITE AND POWDER)

(Stock# 3304)

(February 2000) 304-3

² All chemical names are indexed as complete phrases, individual words, and chemically significant segments of words. Use /FW to restrict retrieval to the complete term, e.g., S ETHANE/FW to only select ethane as a single word rather than as a segment of a larger chemical term, such as trichloroethane.

 $^{^3}$ Searchable as /DP in the Basic Index and using DP= or RP= in the Additional Indexes.

Includes Monograph Name (/MN, MN=), C.A. Names (/CN, CN=), Brand Names (/TN, TN=), Derivative Names (/DERIV), Drug Codes (/SY, SY=), and Synonyms (/SY, SY=).

⁶ Searchable using /TC in the Basic Index and using TC= or TV= in the Additional Indexes.

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ADDITIONAL INDEXES (cont'd)

SEARCH PREFIX	CODE	THE TAXABLE	INDEXING	SELECT EXAMPLES
RE=	RE	Refractive Index ^{1,7}		
RI=	RE	Refractive Index Text ¹	Numeric	S RE=1.0:1.5
RN=	RN	CAS(R) Registry Number	Word	S RI=(D(W)20)
	1	or to (it) registry (duffiber	Phrase	S RN=75847-73-3
	ł			S RN=75847-73-3/MAIN
RP=	RP	References Present ¹		S RN=76095-16-4/DERIV
SO=	so	Releiences Present	Phrase	S RP=PHARMACODYNAMICS
SY=	SY	Bibliographic Sources ⁶	Word	S SO=/FEDCUSON/ON MAMICS
	"	Synonyms Including Brand Names and Drug	Word &	S SO=(FERGUSON(S)J(1W)CLIN(W)PHARMACOL? S SY=INNOVACE
TC=	тс	Louis .	Phrase	O O I MMOVACE
TN=		Therapeutic Category ¹	Word	S SY="1-(N-((S)-1-CARBOXY-3-PHENYLPROPYL"?
TV=	TN	Brand Name ¹	Phrase	O TOTALITATE PROFIVE
	TV	Therapeutic Category (Veterinary) ¹		S TN=INNOVACE
UD=		Update	Word	S TV=(ANABOLIC(W)STEROID
JS=	US	Uses ¹	Phrase	2 OD=3999
JT=	UV	Ultraviolet Maximum Text ¹	Word	S US=(MORDANT(S)LEATHER)
JV=	UV	Ultraviolet Maximum ^{1,7}	Word	S UT=ALCOHOL AND LIV=235
DISPLAY	ONLY	2 May Note: Maximum	Numeric	S UV=260:265
	B1	Boiling Point (Derivative)		
	C1	CA Chaminal N. (Derivative)		
_ I	C2	CA Chemical Name (Derivative)		
_	D1	Company Name (Derivative)		
_	D2	Data Present (Derivative)		
_	FL	Relative Density (Derivative)		
-	L1	Flash Point (Derivative)		
- 1	1	Lethal Dose (LD50) (Derivative)		
1	M1	Molecular Composition(Derivative)		
	IVIZ	Molecular Formula (Derivative)		
-	IVIS	Melting Point (Derivative)		
-	IVI4	Molecular Weight (Derivative)		
	IVIC	Molecular Composition	1	
	וא וא	Chemical Names (Derivative)	1	
	112	Chemical Names, Additional (Derivative)	1	
	∵ ,	Optical Rotation (Derivative)	į	
.	P1	Physical Property Information (Derivative)	ļ	
-	R1	Refractive Index (Derivative)		
	R2	CAS Registry Number (Derivative)		
		Bibliographic Course (Derivative)	- 1	
		Bibliographic Sources (Derivative)	1	
		Synonyms (Derivative)	!	
	, ,	Brand Name (Derivative)	}	
- 1	יאיכ ל	Ultraviolet Maximum (Derivative)	j	

Numeric values can be entered in several different ways: directly as a number, e.g. S BP=100:0; or in exponential notation, e.g. S BP=1E2. Letter abbreviations are also available: K for thousand; M for million, B for billion, e.g. S BP=0.5K:1.0K. To search a range of values, use a colon between starting and ending value, e.g. S BP=78:79 OR use numeric operators (>, <, >=, and <=), e.g. S 78<=BP<=79.

SPECIAL FEATURES

For command descriptions, enter HELP LIMIT, HELP SORT, HELP RANK, HELP MAP online.

1		
LIMIT	/DERIV Information relating to the derivative data mentioned in the monograph /MAIN Information relating to the main monograph substance data	S S2/DERIV
SORT	MF, MN, RN, TC	S S1/MAIN
RANK		SORT S2/ALL/MN PRINT S2/5/1-20/TC
	All phrase- and numeric-indexed fields in the Additional Indexes can be ranked. Other RANK codes include: DE	RANK NA
MAP	MN, NA, PN, RN, SY	RANK BP S4
		MAP RN TEMP S4 MAP SYRN TEMP S3

PREDEFINED FORMAT OPTIONS

NO.	DIALOGWEB FORMAT	RECORD CONTENT
1 2 3 4 5 6 7 8 9 K	Full	DIALOG Accession Number Full Record, except Literature References and Physical Data Full Record, except Physical Data Full Record Full Record Full Record Full Record Full Record DIALOG Accession Number/Monograph Number, Monograph Name, CAS Registry Number, and Molecular Formula Full Record, except Literature References DIALOG Accession Number/Monograph Number, Monograph Name, CAS Registry Number, Molecular Formula, Therapeutic Categories, References Present, Data Present Full Record KWIC (Key Word In Context) displays a window of text; may be used alone or with other formats

OTHER OUTPUT OPTIONS

For an explanation, enter HELP TYPE, HELP UDF, HELP TAG online.

		TO CHANGE.
USER DEFINED FORMATS	Display codes listed in the Search Options tables can be used to customize output.	TYPE S3/MN,MF,MP,BP/1-10
TAG DIRECT RECORD	Output can be displayed with tags identifying each display field.	TYPE S3/3/1-5 TAG
ACCESS	If the accession number of a specific record is known, it can be used to display the record directly.	TYPE 03521/5 DISPLAY 03521/MN,MF,MP PRINT 03521/9

FOR ONLINE HELP:

See HELP FIELDS 304 for searchable fields; HELP FORMAT 304 for output formats; HELP LIMIT 304 for limits; HELP RATES 304 for cost information; HELP SORT 304 for sorts.

